Models with Linear Algebraic Equations (Material balances with and without chemical reactions)

- Plant wide or section wide mass balances are accomplish with design stage or later during operation for keeping material audit. Typical example are shown as:

EXAMPLE 1

Recovery of acetone from acetone –air mixture is obtained using an absorber and a flash separator which is single equilibrium stage (Figure).

A model for this system is developed under following assumption

- Air entering the absorber contains no water vapor
- Air leaving the absorber contains 6 mass % water vapor
- All acetone is absorbed in water

  $y = 20.5x$

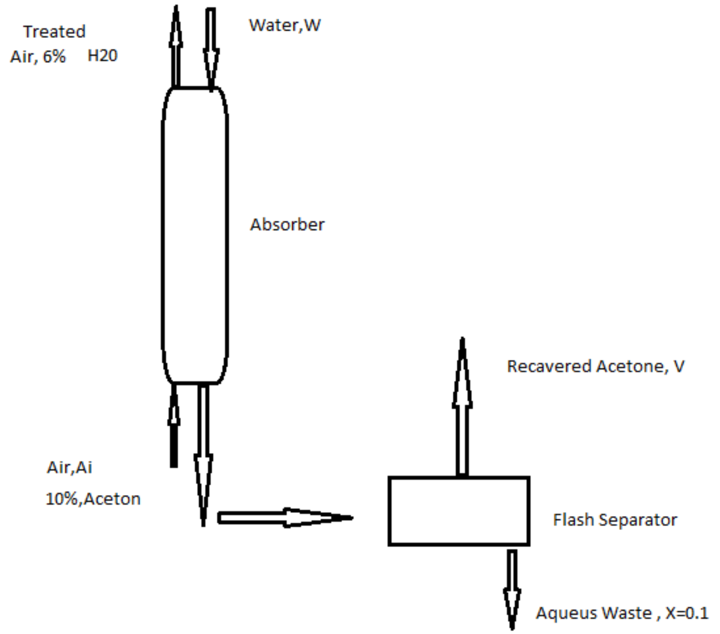


Figure . Flash Drum: Schematic Diagram

Where y mass fraction of the acetone in the vapor stream and x mass fraction of the acetone in the liquid stream (flash separator) .

Operating conditions of the process are as follows

- Air in flow: 800 lb /hr with 10 mass % acetone
- Water flow rate: 400 lb/hr

Mass Balance for air, aseton and water respectively

0.9*Air = 0.94Ao

0.1Ai = 0.04L + y V

Water = 0.06Ao + (1 − y)V + 0.96L

Design requirement : $x = 0.04$; Equilibrium Relation: $y = 20.5\,x$; $\Rightarrow y$

$= 20.5 \times 0.04 = 0.82$

Substituting for all the known values and rearranging, we have the above model is a typical example of system of linear algebraic equations, which have to be solved simultaneously.
$Ax = b$; where x and b are a (n×1) vectors (i.e. $x, b \in Rn$) and A is a (n×n) matrix.

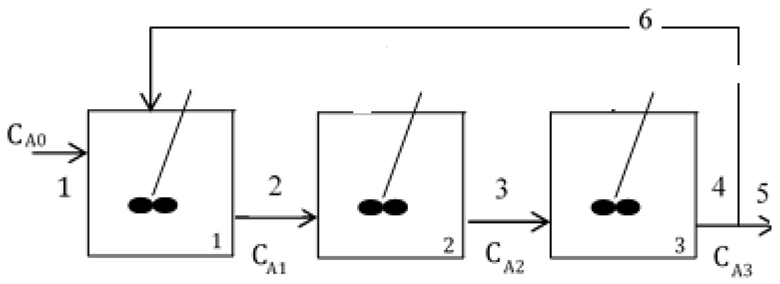
```
>> A=[0.94 0 0 ;0 0.04 0.82;0.06 0.96 0.18]

A =

    0.9400         0         0
         0    0.0400    0.8200
    0.0600    0.9600    0.1800

>> B=[0.9*800;0.1*800;400]

B =

   720
    80
   400

>> x=inv(A)*B

x =

  765.9574
  353.7370
   80.3055
```

EXAMPLE 2

irreversible reaction A→B

$r_A = k.C_A$

$k = 3x10^5 \exp(\frac{-4200}{T}) \quad k[=]\frac{1}{h} \quad T[=]K$



Reactor no	Temperature (°C)	Volume (L)
1	45	700
2	60	1000
3	70	1100

Stream no	Volumetric flowrate (L/h)
1	500
6	200

Determine the concentration of species of A in each reactor if the feed to the first reactor contains 1 mol/L of A.

Finding flow rates, using total mass balance

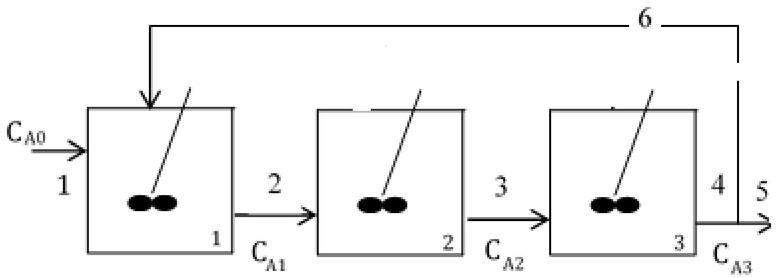
Stream no	1	2	3	4	5	6
Flowrates, L/h	500	700	700	700	500	200

$$Q_1 = Q_5$$

$$Q_5 + Q_6 = Q4$$

$$Q_1 + Q_6 = Q_2$$

$$Q_2 = Q_3 = Q_4$$



$$k_1 = 3x10^5 \exp(\frac{-4200}{45+273}) = 0.551\, h^{-1}$$

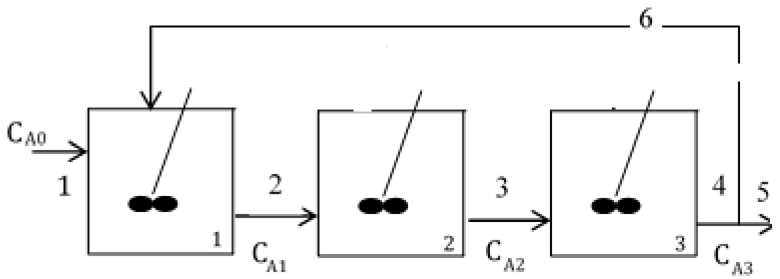
$$k_2 = 3x10^5 \exp(\frac{-4200}{60+273}) = 0.999\, h^{-1}$$

$$k_3 = 3x10^5 \exp(\frac{-4200}{70+273}) = 1.443\, h^{-1}$$

Mass Balance:

Tank 1

$$Q_1 C_{A0} + Q_6 C_{A3} - k_1 C_{A1} V_1 = 0$$



Tank 2

$$Q_2 C_{A1} - Q_3 C_{A2} - k_2 C_{A2} V_2 = 0$$

Tank 3

$$Q_3 C_{A2} - Q_4 C_{A3} - k_3 C_{A3} V_3 = 0$$

$$\begin{bmatrix} -385.7 & 0 & 200 \\ 700 & -1699 & 0 \\ 0 & 700 & -2287.3 \end{bmatrix} \begin{bmatrix} C_{A1} \\ C_{A2} \\ C_{A3} \end{bmatrix} = \begin{bmatrix} -500 \\ 0 \\ 0 \end{bmatrix}$$

```
>> a=[-387.5 0 200;700 -1699 0;0 700 -2287.3]

>> b=[  -500;  0;   0]

>> x=inv(a)*b

x =

   1.3801 (CA1)
   0.5686 (CA2)
   0.1740 (CA3)
```